

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	4	AUG 13	CA/Caplus enhanced with additional kind codes for granted patents
NEWS	5	AUG 20	CA/Caplus enhanced with CAS indexing in pre-1907 records
NEWS	6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	7	AUG 27	USPATOLD now available on STN
NEWS	8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	10	SEP 13	FORIS renamed to SOFIS
NEWS	11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	12	SEP 17	CA/Caplus enhanced with printed CA page images from 1967-1998
NEWS	13	SEP 17	Caplus coverage extended to include traditional medicine patents
NEWS	14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	15	OCT 02	CA/Caplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	16	OCT 19	BEILSTEIN updated with new compounds
NEWS	17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	18	NOV 19	WPIX enhanced with XML display format
NEWS	19	NOV 30	ICSD reloaded with enhancements
NEWS	20	DEC 04	LINPADOCDB now available on STN
NEWS	21	DEC 14	BEILSTEIN pricing structure to change
NEWS	22	DEC 17	USPATOLD added to additional database clusters
NEWS	23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	24	DEC 17	DGENE now includes more than 10 million sequences
NEWS	25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS	27	DEC 17	CA/Caplus enhanced with new custom IPC display formats
NEWS	28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	29	JAN 02	STN pricing information for 2008 now available
NEWS	30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	32	JAN 28	MARPAT searching enhanced
NEWS	33	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	34	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment

NEWS 35 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 36 FEB 08 STN Express, Version 8.3, now available

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 24 JANUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 18:57:40 ON 19 FEB 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 18:58:17 ON 19 FEB 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7
DICTIONARY FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

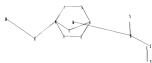
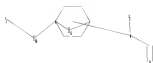
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10518714c.str



```

chain nodes :
11 12 13 15 17 18
ring nodes :
1 2 3 4 5 6 7
chain bonds :
4-17 11-12 11-15 12-13 17-18
ring bonds :
1-2 1-6 1-7 2-3 3-4 4-5 4-7 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-7 4-17 5-6 11-12 11-15 12-13 17-18
exact bonds :
1-7
isolated ring systems :
containing 1 :
```

G1:H,Ak

G2:C,O,S,N

```

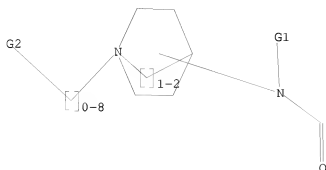
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 11:CLASS 12:CLASS
13:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
```

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 H,Ak

G2 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 18:58:37 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 90592 TO ITERATE

2.2% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 1793956 TO 1829724

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 18:58:42 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1812585 TO ITERATE

54.1% PROCESSED 981134 ITERATIONS

173 ANSWERS

55.2% PROCESSED 1000000 ITERATIONS

173 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.24

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 1812585 TO 1812585

PROJECTED ANSWERS: 260 TO 366

L3 173 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY
178.82

SESSION
179.03

FILE 'CAPLUS' ENTERED AT 18:59:16 ON 19 FEB 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 19 Feb 2008 VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008 (20080218/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

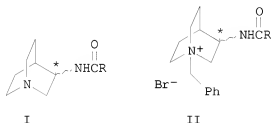
<http://www.cas.org/infopolicy.html>

=> s l3 full

L4 6 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:849820 CAPLUS
 DOCUMENT NUMBER: 147:211644
 TITLE: 3-amidoquinuclidine derivatives: synthesis and interaction with butyrylcholinesterase
 AUTHOR(S): Odzak, Renata; Primozic, Ines; Tomic, Srdanka
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Zagreb, Zagreb, HR-10000, Croatia
 SOURCE: Croatica Chemica Acta (2007), 80(1), 101-107
 CODEN: CCACAA; ISSN: 0011-1643
 PUBLISHER: Croatian Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 147:211644
 GI

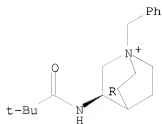


AB Racemates as well as (R)- and (S)-enantiomers of 3-pivalamidoquinuclidine I (R = Me₃C) and 3-acetamidoquinuclidine I (R = Me) were prepared. Their quaternary racemic and enantiomerically pure N-benzyl derivs. II (R = Me₃C, Me) were synthesized as well. I and II were tested as substrates and inhibitors of butyrylcholinesterase (BChE) from horse serum (EC 3.1.1.8). No hydrolysis was observed under the exptl. conditions applied. On the contrary, inhibition of BChE by (R)- and (S)-enantiomers of II (R = Me₃C) was observed. II (R = Me₃C) with K_i = 41.57 μmol dm⁻³ was a 3-fold more potent inhibitor than the (R)-enantiomer. On the other hand, preliminary results indicated that both enantiomers of II (R = Me) may possibly be inhibitors as well as activators depending on the concns. of benzoylcholine (BzCh) used as a substrate of BChE.

IT 945216-82-0P 945216-83-1P 945216-85-3P
 945216-86-4P
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
 SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of racemic and enantiopure quaternary N-benzylamidoquinuclidines from 3-aminoquinuclidine and acid anhydrides and their interaction with butyrylcholinesterase)

RN 945216-82-0 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[(2,2-dimethyl-1-oxopropyl)amino]-1-(phenylmethyl)-, bromide (1:1), (3R)- (CA INDEX NAME)

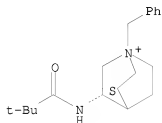
Absolute stereochemistry. Rotation (+).



RN 945216-83-1 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(2,2-dimethyl-1-oxopropyl)amino]-1-(phenylmethyl)-, bromide (1:1), (3S)- (CA INDEX NAME)

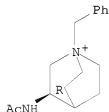
Absolute stereochemistry. Rotation (-).



RN 945216-85-3 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-(acetylamino)-1-(phenylmethyl)-, bromide (1:1), (3R)- (CA INDEX NAME)

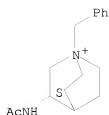
Absolute stereochemistry. Rotation (+).



RN 945216-86-4 CAPLUS

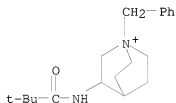
CN 1-Azoniabicyclo[2.2.2]octane, 3-(acetylamino)-1-(phenylmethyl)-, bromide (1:1), (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



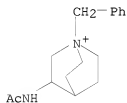
● Br⁻

IT 945216-81-9P 945216-84-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of racemic and enantiopure quaternary N-benzylamidoquinuclidines from 3-aminoquinuclidine and acid anhydrides and their interaction with butyrylcholinesterase)
 RN 945216-81-9 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[(2,2-dimethyl-1-oxopropyl)amino]-1-(phenylmethyl)-, bromide (1:1) (CA INDEX NAME)



● Br⁻

RN 945216-84-2 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-(acetylamino)-1-(phenylmethyl)-, bromide (1:1) (CA INDEX NAME)



● Br⁻

REFERENCE COUNT:

18

THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:384736 CAPLUS

DOCUMENT NUMBER: 146:402148

TITLE: Preparation of azabicyclic derivatives of indazoles, benzothiazoles, benzisothiazoles, benzisoxazoles, pyrazolopyridines, isothiazolopyridines for therapeutic use as $\alpha 7$ -nACh receptor activators

INVENTOR(S): Schumacher, Richard; Danca, Mihaela Diana; Ma, Jianguo; Herbert, Brian; Nguyen, Truc Minh; Xie, Wenge; Tehim, Ashok

PATENT ASSIGNEE(S): Memory Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 283pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

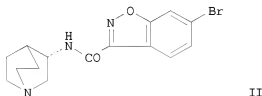
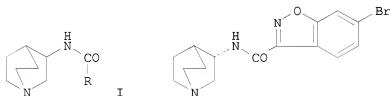
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007038367	A1	20070405	WO 2006-US37142	20060922
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW</p> <p>RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p>				
US 2007078147	A1	20070405	US 2006-525213	20060922
PRIORITY APPLN. INFO.:			US 2005-719552P	P 20050923
			US 2006-791881P	P 20060414

OTHER SOURCE(S): MARPAT 146:402148

GI



AB N-azabicyclo[2.2.2]octyl-heterocyclic amide derivs., such as I [R = heterocyclyl, such as those cited in the title], were prepared as $\alpha 7$ nicotinic acetylcholine receptor ($\alpha 7$ -nAChR) ligands which activate or enhance defective or malfunctioning nAChR activity, especially of the brain, and are useful in the treatment of psychotic disease, neurodegenerative disease and conditions of memory and/or cognition impairment. These diseases and conditions may include schizophrenia, anxiety, mania, depression, manic depression, Tourette's syndrome, Parkinson's disease, Huntington's disease, Alzheimer's disease, Lewy body dementia, amyotrophic lateral sclerosis, memory impairment, memory loss, cognition deficit,

attention deficit, attention deficit hyperactivity disorder (ADHD) and mild cognitive impairment due to aging, Alzheimer's disease, schizophrenia, Parkinson's disease, Huntington's disease, Pick's disease, Creutzfeldt-Jakob disease, depression, aging, head trauma, stroke, CNS hypoxia, cerebral senility, multiinfarct dementia, HIV and/or cardiovascular disease. These diseases may further include alc. and nicotine addiction, pain, jet lag, obesity, diabetes, vascular dementia (VaD), age-associated cognitive decline (AACD), amnesia associated with open-heart-surgery, cardiac arrest, general anesthesia, memory deficits from exposure to anesthetic agents, sleep deprivation induced cognitive impairment, chronic fatigue syndrome, narcolepsy, AIDS-related dementia, epilepsy-related cognitive impairment, Down's syndrome, alcoholism related dementia, drug/substance induced memory impairments and dementia puglistica (boxer syndrome). Thus, amide II was prepared via an amidation reaction of (3S)-3-aminoquinuclidine hydrochloride with Et 6-bromobenzisoxazole-3-carboxylate in EtOH using N,N-diisopropylethylamine. The prepared amides were assayed for $\alpha 7$ -nAChR binding affinity.

IT 932705-66-3P 932705-69-6P

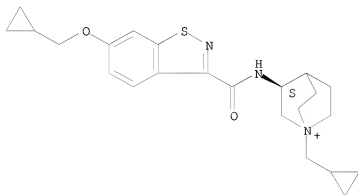
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of azabicyclic derivs. of indazoles, benzothiazoles, benzisothiazoles, benzisoxazoles, pyrazolopyridines, isothiazolopyridines for therapeutic use as $\alpha 7$ -nACh receptor activators)

RN 932705-66-3 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[6-(cyclopropylmethoxy)-1,2-benzisothiazol-3-yl]carbonyl]amino]-1-(cyclopropylmethyl)-, bromide (1:1), (3S)- (CA INDEX NAME)

Absolute stereochemistry.

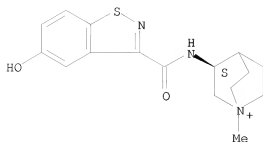


● Br⁻

RN 932705-69-6 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[5-hydroxy-1,2-benzisothiazol-3-yl]carbonyl]amino]-1-methyl-, iodide (1:1), (3S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 932703-96-3P 932704-00-2P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azabicyclic derivs. of indazoles, benzothiazoles, benzoisothiazoles, benzisoxazoles, pyrazolopyridines, isothiazolopyridines for therapeutic use as α 7-nACh receptor activators)

RN 932703-96-3 CAPLUS

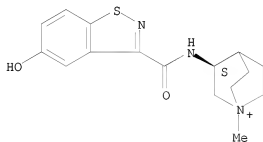
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[5-hydroxy-1,2-benzisothiazol-3-yl]carbonyl]amino]-1-methyl-, formate (1:1), (3S)- (CA INDEX NAME)

CM 1

CRN 932703-95-2

CMF C16 H20 N3 O2 S

Absolute stereochemistry.



CM 2

CRN 71-47-6

CMF C H O2

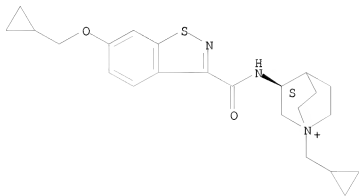


RN 932704-00-2 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[6-(cyclopropylmethoxy)-1,2-benzisothiazol-3-yl]carbonyl]amino]-1-(cyclopropylmethyl)-, formate (1:1), (3S)- (CA INDEX NAME)

CM 1
CRN 932703-99-6
CMF C23 H30 N3 O2 S

Absolute stereochemistry.

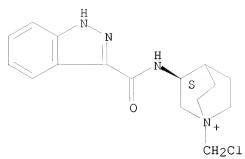


CM 2
CRN 71-47-6
CMF C H O2

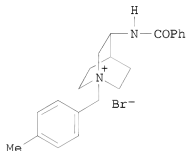


IT 932705-49-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of azabicyclic derivs. of indazoles, benzothiazoles,
benzothiazoles, benzisoxazoles, pyrazolopyridines,
isothiazolopyridines for therapeutic use as α 7-nACh receptor
activators)
RN 932705-49-2 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-(chloromethyl)-3-[(1H-indazol-3-
ylcarbonyl)amino]-, chloride (1:1), (3S)- (CA INDEX NAME)

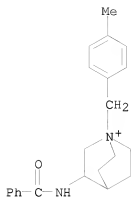
Absolute stereochemistry.



L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:1091765 CAPLUS
 DOCUMENT NUMBER: 146:27960
 TITLE: Synthesis of new N-quaternary-3-benzamidoquinuclidinium salts
 AUTHOR(S): Odzak, Renata; Tomic, Srdjanka
 CORPORATE SOURCE: Department of Chemistry, Faculty of Natural Sciences, Mathematics and Education, University of Split, Split, 21 000, Croatia
 SOURCE: Molecules (2006), 11(9), 726-730
 CODEN: MOLEFW; ISSN: 1420-3049
 URL: <http://www.mdpi.org/molecules/papers/11090726.pdf>
 PUBLISHER: Molecular Diversity Preservation International
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 146:27960
 GI



- AB The synthesis of racemic and enantiomerically pure N-p-methylbenzyl and N-p-chlorobenzylbenzamidoquinuclidinium bromides, e.g., I, is described. These compds. were prepared from racemic or enantiomerically pure 3-benzamidoquinuclidines using the appropriate quaternization reagents: p-methyl-benzyl bromide and p-chlorobenzyl bromide.
 IT 915207-68-0P 915207-69-1P 915207-70-4P
 915207-71-5P 915207-72-6P 915207-73-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of racemic/enantiopure quaternary benzylbenzamidoquinuclidinium derivs. by quaternization of racemic/enantiopure benzamidoquinuclidines with methyl/chlorobenzyl bromides)
 RN 915207-68-0 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-[(4-methylphenyl)methyl]-, bromide (1:1) (CA INDEX NAME)

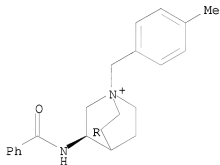


● Br⁻

RN 915207-69-1 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-[(4-methylphenyl)methyl]-, bromide (1:1), (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

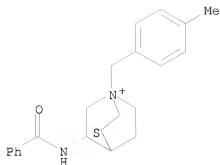


● Br⁻

RN 915207-70-4 CAPLUS

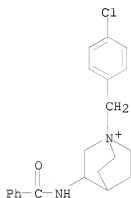
CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-[(4-methylphenyl)methyl]-, bromide (1:1), (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 915207-71-5 CAPLUS

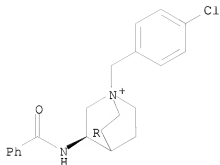
CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-[(4-chlorophenyl)methyl]-, bromide (1:1) (CA INDEX NAME)



RN 915207-72-6 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-[(4-chlorophenyl)methyl]-, bromide (1:1), (3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

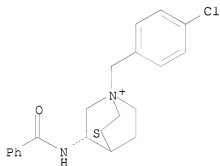


● Br⁻

RN 915207-73-7 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-[(4-chlorophenyl)methyl]-, bromide (1:1), (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



● Br⁻

REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:285227 CAPLUS

DOCUMENT NUMBER: 144:480386

TITLE: 3-Amidoquinuclidine derivatives: Synthesis of compounds and inhibition of butyrylcholinesterase

AUTHOR(S): Odzak, Renata; Tomic, Srdanka

CORPORATE SOURCE: Laboratory of Organic Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Zagreb, HR-10 000, Croatia

SOURCE: Bioorganic Chemistry (2006), 34(2), 90-98

CODEN: BOCMBM; ISSN: 0045-2068

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:480386

AB The synthesis of racemic and enantiomerically pure 3-butanamidoquinuclidines ((±)-Bu, (R)-Bu and (S)-Bu), (1-3) and 3-benzamidoquinuclidines ((±)-Bz, (R)-Bz, and (S)-Bz), (4-6) is described. The N-quaternary derivs., N-benzyl-3-butanamidoquinuclidinium bromides ((±)-Bn1Bu, (R)-Bn1Bu and (S)-Bn1Bu), (7-9) and N-benzyl-3-benzamidoquinuclidinium bromides ((±)-Bn1Bz, (R)-Bn1Bz and (S)-Bn1Bz), (10-12) were subsequently synthesized. The interaction of the four enantiomerically pure quaternary derivs. with horse serum butyrylcholinesterase (BChE) was tested. All tested compds. inhibited the enzyme. The best inhibitor of the enzyme was (S)-Bn1Bz with a $K_i = 3.7 \mu\text{M}$. The inhibitor potency decreases in order (S)-Bn1Bz > (R)-Bn1Bz > (R)-Bn1Bu > (S)-Bn1Bu.

IT 887150-91-6P 887150-92-7P 887150-93-8P

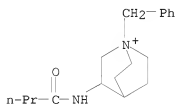
887150-94-9P 887150-95-0P 887150-96-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(amidoquinuclidine derivs. as inhibitors of butyrylcholinesterase)

RN 887150-91-6 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(1-oxobutyl)amino]-1-(phenylmethyl)-, bromide (9CI) (CA INDEX NAME)

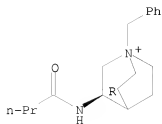


● Br⁻

RN 887150-92-7 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(1-oxobutyl)amino]-1-(phenylmethyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

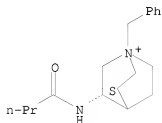


● Br⁻

RN 887150-93-8 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(1-oxobutyl)amino]-1-(phenylmethyl)-, bromide, (3S)- (9CI) (CA INDEX NAME)

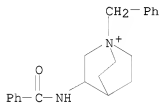
Absolute stereochemistry. Rotation (-).



● Br⁻

RN 887150-94-9 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-(phenylmethyl)-, bromide (9CI) (CA INDEX NAME)

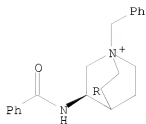


● Br⁻

RN 887150-95-0 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-(phenylmethyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

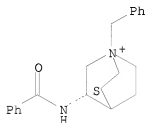


● Br⁻

RN 887150-96-1 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-(benzoylamino)-1-(phenylmethyl)-, bromide,
(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



● Br⁻

REFERENCE COUNT:

24

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:41467 CAPLUS

DOCUMENT NUMBER: 140:94180

TITLE: Preparation of new quinuclidine amide derivatives for therapeutic uses as antagonists of M3 muscarinic receptors

INVENTOR(S): Prat Quinones, Maria

PATENT ASSIGNEE(S): Almirall Prodesfarma S.A., Spain

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

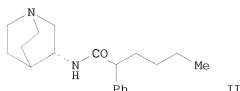
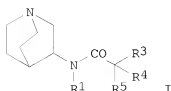
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005285	A1	20040115	WO 2003-EP6708	20030625
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, IJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
ES 2204295	A1	20040416	ES 2002-1539	20020702
ES 2204295	B1	20050801		
CA 2492535	A1	20040115	CA 2003-2492535	20030625
AU 2003242757	A1	20040123	AU 2003-242757	20030625
EP 1519933	A1	20050406	EP 2003-762514	20030625
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2003012216	A	20050412	BR 2003-12216	20030625
CN 1678610	A	20051005	CN 2003-820648	20030625
JP 2005533826	T	20051110	JP 2004-518575	20030625
NZ 537341	A	20060428	NZ 2003-537341	20030625
RU 2314306	C2	20080110	RU 2005-102585	20030625
MX 2004PA12271	A	20050408	MX 2004-PA12271	20041207
ZA 2004010404	A	20050905	ZA 2004-10404	20041223
IN 2004DN041140	A	20061229	IN 2004-DN4140	20041227
NO 2005000164	A	20050404	NO 2005-164	20050112
US 2006167042	A1	20060727	US 2005-518714	20050801

PRIORITY APPLN. INFO.:

ES 2002-1539 A 20020702
WO 2003-EP6708 W 20030625

OTHER SOURCE(S): MARPAT 140:94180

GI



AB N-quinuclidinyl amides, such as I [R1 = H, alkyl; R3 = furyl, thienyl, phenyl; R4 = alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylmethyl, Ph,

benzyl, phenethyl, furyl, thienyl; R5 = H, OH, Me, CH2OH], were prepared for use in therapy as antagonists of M3 muscarinic receptors. These amides are claimed for use in the treatment of respiratory, urol. or gastrointestinal pathol. conditions and diseases susceptible to amelioration by antagonism of M3 muscarinic receptors. Thus, amide II was prepared in 63.1% yield via an amidation reaction of (3R)-aminoquinuclidine with 2-phenylhexanoic acid in DMF and CHCl3. The prepared N-quinuclidinyl amides were assayed for human muscarinic receptor binding activity and for effect on bronchial response to i.v. acetylcholine challenge in guinea pigs. Tablet, liquid inhalant, powder inhalant, and inhalation aerosol pharmaceutical compns. of the amides were presented.

IT 644468-34-8P 644468-36-0P 644468-39-3P
 644468-42-8P 644468-45-1P 644468-46-2P
 644468-48-4P 644468-50-8P 644468-52-0P
 644468-53-1P 644468-55-3P 644468-56-4P
 644468-57-5P 644468-59-7P 644468-60-0P
 644468-62-2P 644468-72-4P 644468-73-5P
 644468-75-7P 644468-77-9P 644468-79-1P
 644468-80-4P 644468-82-6P 644468-84-8P
 644468-85-9P 644468-86-0P 644468-87-1P
 644468-88-2P 644468-89-3P 644468-90-6P
 644468-91-7P 644468-92-8P 644468-93-9P
 644468-94-0P 644468-95-1P 644468-96-2P
 644468-97-3P 644468-99-5P 644469-01-2P
 644469-03-4P 644469-05-6P 644469-07-8P
 644469-08-9P

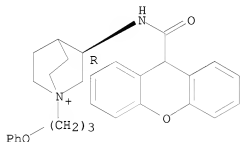
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-quinuclidinyl amides for use in pharmaceutical compns. as M3 muscarinic receptor antagonists)

RN 644468-34-8 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 1-(3-phenoxypropyl)-3-[(9H-xanthen-9-yl)carbonyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

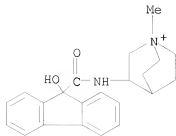
Absolute stereochemistry.



● Br⁻

RN 644468-36-0 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[9-hydroxy-9H-fluoren-9-yl)carbonyl]amino]-1-methyl-, bromide (9CI) (CA INDEX NAME)



RN 644468-39-3 CAPLUS

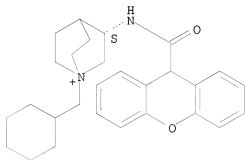
CN 1-Azoniabicyclo[2.2.2]octane, 1-(cyclohexylmethyl)-3-[(9H-xanthen-9-ylcarbonyl)amino]-, (3S)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-38-2

CMF C28 H35 N2 O2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

CMF C2 F3 O2



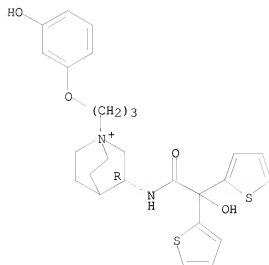
RN 644468-42-8 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[3-(3-hydroxyphenoxy)propyl]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-41-7
 CMF C26 H31 N2 O4 S2

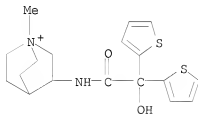
Absolute stereochemistry.



CM 2
 CRN 14477-72-6
 CMF C2 F3 O2

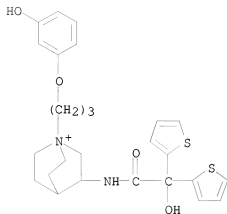


RN 644468-45-1 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-methyl-, bromide (9CI) (CA INDEX NAME)



RN 644468-46-2 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[3-(3-

hydroxyphenoxy)propyl]-, bromide (9CI) (CA INDEX NAME)



RN 644468-48-4 CAPLUS

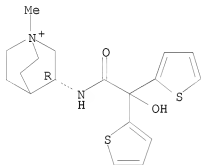
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-methyl-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-47-3

CMF C18 H23 N2 O2 S2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

CMF C2 F3 O2



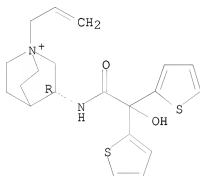
RN 644468-50-8 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(2-propenyl)-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-49-5

CMF C20 H25 N2 O2 S2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

CMF C2 F3 O2



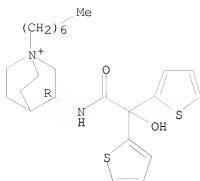
RN 644468-52-0 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 1-heptyl-3-[(hydroxydi-2-thienylacetyl)amino]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-51-9

CMF C24 H35 N2 O2 S2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

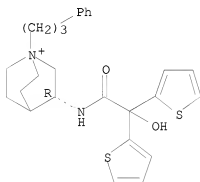
CMF C2 F3 O2



RN 644468-53-1 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(3-phenylpropyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



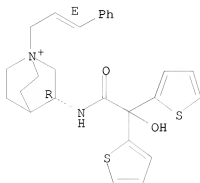
RN 644468-55-3 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[(2E)-3-phenyl-2-propenyl]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-54-2
 CMF C26 H29 N2 O2 S2

Absolute stereochemistry.
 Double bond geometry as shown.

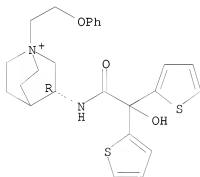


CM 2
 CRN 14477-72-6
 CMF C2 F3 O2



RN 644468-56-4 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(2-phenoxyethyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

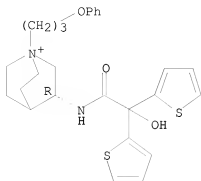
Absolute stereochemistry.



RN 644468-57-5 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(3-

phenoxypropyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br⁻

RN 644468-59-7 CAPLUS

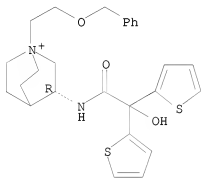
CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[2-(phenylmethoxy)ethyl]-, (3R)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-58-6

CMF C26 H31 N2 O3 S2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

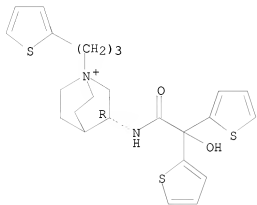
CMF C2 F3 O2



RN 644468-60-0 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-[3-(2-thienyl)propyl]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

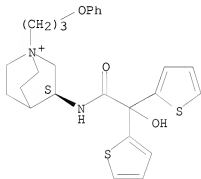


● Br⁻

RN 644468-62-2 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(hydroxydi-2-thienylacetyl)amino]-1-(3-phenoxypropyl)-, bromide, (3S)- (9CI) (CA INDEX NAME)

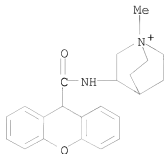
Absolute stereochemistry.



● Br⁻

RN 644468-72-4 CAPLUS

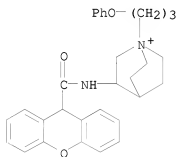
CN 1-Azoniabicyclo[2.2.2]octane, 1-methyl-3-[(9H-xanthen-9-ylcarbonyl)amino]-, bromide (9CI) (CA INDEX NAME)



● Br⁻

RN 644468-73-5 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 1-(3-phenoxypropyl)-3-[(9H-xanthen-9-ylcarbonyl)amino]-, bromide (9CI) (CA INDEX NAME)



● Br⁻

RN 644468-75-7 CAPLUS

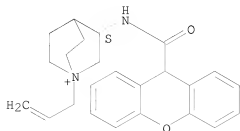
CN 1-Azoniabicyclo[2.2.2]octane, 1-(2-propenyl)-3-[(9H-xanthen-9-ylcarbonyl)amino]-, (3S)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-74-6

CMF C24 H27 N2 O2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

CMF C2 F3 O2



RN 644468-77-9 CAPLUS

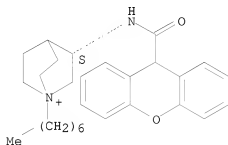
CN 1-Azoniabicyclo[2.2.2]octane, 1-heptyl-3-[(9H-xanthen-9-ylcarbonyl)amino]-, (3S)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-76-8

CMF C28 H37 N2 O2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

CMF C2 F3 O2



RN 644468-79-1 CAPLUS

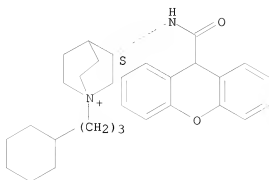
CN 1-Azoniabicyclo[2.2.2]octane, 1-(3-cyclohexylpropyl)-3-[(9H-xanthen-9-ylcarbonyl)amino]-, (3S)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-78-0

CMF C30 H39 N2 O2

Absolute stereochemistry.



CM 2

CRN 14477-72-6

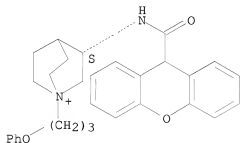
CMF C2 F3 O2



RN 644468-80-4 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 1-(3-phenoxypropyl)-3-[(9H-xanthen-9-ylcarbonyl)amino]-, bromide, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br⁻

RN 644468-82-6 CAPLUS

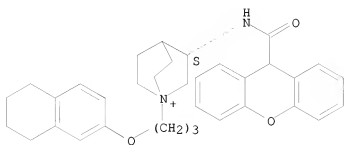
CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-[(5,6,7,8-tetrahydro-2-naphthalenyl)oxy]propyl]-3-[(9H-xanthen-9-ylcarbonyl)amino]-, (3S)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-81-5

CMF C34 H39 N2 O3

Absolute stereochemistry.



CM 2

CRN 14477-72-6

CMF C2 F3 O2



RN 644468-84-8 CAPLUS

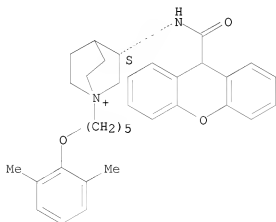
CN 1-Azoniabicyclo[2.2.2]octane, 1-[5-(2,6-dimethylphenoxy)pentyl]-3-[(9H-xanthen-9-ylcarbonyl)amino]-, (3S)-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 644468-83-7

CMF C34 H41 N2 O3

Absolute stereochemistry.

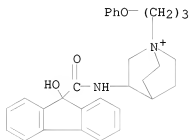


CM 2

CRN 14477-72-6
CMF C2 F3 O2

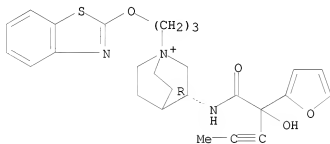


RN 644468-85-9 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[(9-hydroxy-9H-fluoren-9-yl)carbonyl]amino]-1-(3-phenoxypropyl)-, bromide (9CI) (CA INDEX NAME)



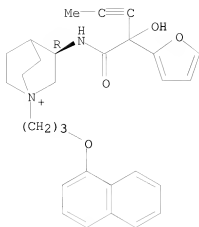
RN 644468-86-0 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-(2-benzothiazolyloxy)propyl]-3-[[2-(2-furanyl)-2-hydroxy-1-oxo-3-pentynyl]amino]-, chloride, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



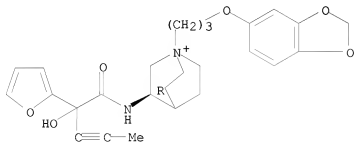
RN 644468-87-1 CAPLUS
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[2-(2-furanyl)-2-hydroxy-1-oxo-3-pentynyl]amino]-1-[3-(1-naphthalenyloxy)propyl]-, chloride, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



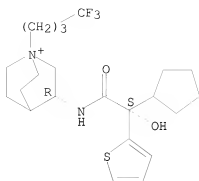
RN 644468-88-2 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-(1,3-benzodioxol-5-yloxy)propyl]-3-[[2-(2-furanyl)-2-hydroxy-1-oxo-3-pentynyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 644468-89-3 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[[2-(2S)-cyclopentylhydroxy-2-thienylacetyl]amino]-1-(4,4,4-trifluorobutyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

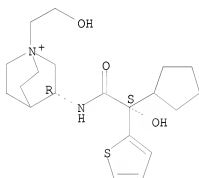
Absolute stereochemistry.



● Br⁻

RN 644468-90-6 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[(2S)-cyclopentylhydroxy-2-thienylacetyl]amino]-1-(2-hydroxyethyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

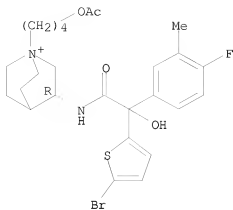
Absolute stereochemistry.



● Br⁻

RN 644468-91-7 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 1-[4-(acetyloxy)butyl]-3-[[[(5-bromo-2-thienyl)(4-fluoro-3-methylphenyl)hydroxyacetyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

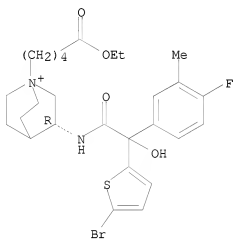
Absolute stereochemistry.



● Br⁻

RN 644468-92-8 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[(5-bromo-2-thienyl)(4-fluoro-3-methylphenyl)hydroxyacetyl]amino]-1-(5-ethoxy-5-oxopentyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

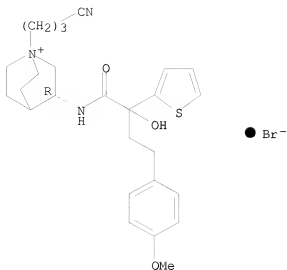
Absolute stereochemistry.



● Br⁻

RN 644468-93-9 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 1-(3-cyanopropyl)-3-[[[2-hydroxy-4-(4-methoxyphenyl)-1-oxo-2-(2-thienyl)butyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

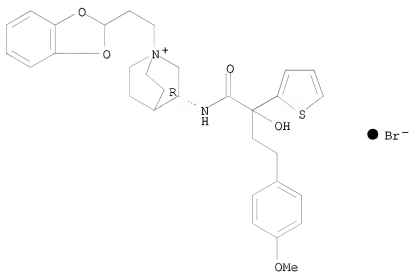
Absolute stereochemistry.



RN 644468-94-0 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 1-[2-(1,3-benzodioxol-2-yl)ethyl]-3-[[2-hydroxy-4-(4-methoxyphenyl)-1-oxo-2-(2-thienyl)butyl]amino]-, bromide, (3R)- (9CI) (CA INDEX NAME)

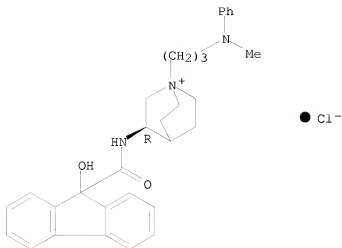
Absolute stereochemistry.



RN 644468-95-1 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[(9-hydroxy-9H-fluoren-9-yl)carbonyl]amino]-1-[3-(methylphenylamino)propyl]-], chloride, (3R)- (9CI) (CA INDEX NAME)

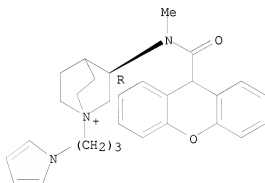
Absolute stereochemistry.



RN 644468-96-2 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[methyl(9H-xanthen-9-ylcarbonyl)amino]-1-[3-(1H-pyrrol-1-yl)propyl]-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

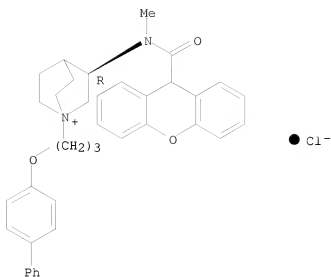


● Br⁻

RN 644468-97-3 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-([1,1'-biphenyl]-4-yloxy)propyl]-3-[methyl(9H-xanthen-9-ylcarbonyl)amino]-, chloride, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

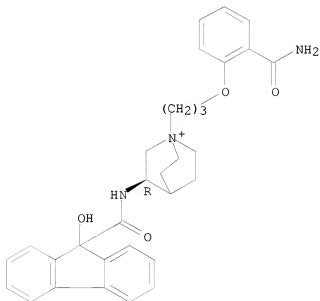


RN 644468-99-5 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-[2-(aminocarbonyl)phenoxy]propyl]-3-[[9-hydroxy-9H-fluoren-9-yl]carbonyl]amino]-, (3R)-, formate (salt) (9CI)
 (CA INDEX NAME)

CM 1

CRN 644468-98-4
 CMF C31 H34 N3 O4

Absolute stereochemistry.



CM 2

CRN 71-47-6
 CMF C H O2

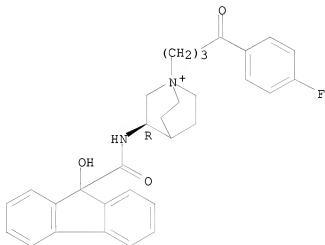


RN 644469-01-2 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 1-[4-(4-fluorophenyl)-4-oxobutyl]-3-[[9-hydroxy-9H-fluoren-9-yl)carbonyl]amino]-, (3R)-, formate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 644469-00-1
 CMF C31 H32 F N2 O3

Absolute stereochemistry.



CM 2

CRN 71-47-6
 CMF C H O2

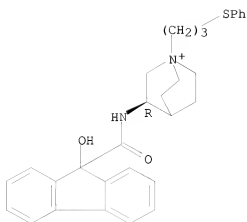


RN 644469-03-4 CAPLUS
 CN 1-Azoniabicyclo[2.2.2]octane, 3-[[9-hydroxy-9H-fluoren-9-yl)carbonyl]amino]-1-[3-(phenylthio)propyl]-, (3R)-, formate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 644469-02-3
 CMF C30 H33 N2 O2 S

Absolute stereochemistry.



CM 2

CRN 71-47-6

CMF C H O2



RN 644469-05-6 CAPLUS

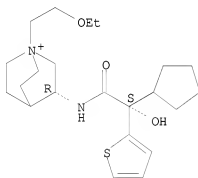
CN 1-Azoniabicyclo[2.2.2]octane, 3-[[(2S)-cyclopentylhydroxy-2-thienylacetyl]amino]-1-(2-ethoxyethyl)-, (3R)-, formate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 644469-04-5

CMF C22 H35 N2 O3 S

Absolute stereochemistry.



CM 2

CRN 71-47-6

CMF C H O2



RN 644469-07-8 CAPLUS

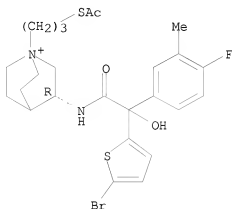
CN 1-Azoniabicyclo[2.2.2]octane, 1-[3-(acetylthio)propyl]-3-[[5-bromo-2-thienyl](4-fluoro-3-methylphenyl)hydroxyacetyl]amino]-, (3R)-, formate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 644469-06-7

CMF C25 H31 Br F N2 O3 S2

Absolute stereochemistry.



CM 2

CRN 71-47-6

CMF C H O2



RN 644469-08-9 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[(di-2-thienylacetyl)amino]-1-(3-phenoxypropyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:991508 CAPLUS

DOCUMENT NUMBER: 140:42022

TITLE: Preparation of 2-heteroaryl carboxamides for the treatment and/or the prophylaxis of diseases effecting memory

INVENTOR(S): Luithle, Joachim; Boess, Frank-Gerhard; Erb, Christina; Hafner, Frank-Thorsten; Schnizler, Katrin; Flessner, Timo; Van Kampen, Marja; Van Der Staay, Franz-Josef

PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany

SOURCE: PCT Int. Appl., 239 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

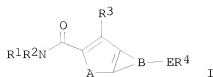
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

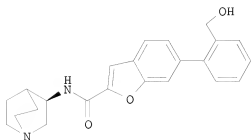
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003104227	A1	20031218	WO 2003-EP5735	20030602
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10257078	A1	20040624	DE 2002-10257078	20021206
DE 10257537	A1	20040701	DE 2002-10257537	20021210
DE 10305922	A1	20040304	DE 2003-10305922	20030213
CA 2488761	A1	20031218	CA 2003-2488761	20030602
AU 2003238450	A1	20031222	AU 2003-238450	20030602
EP 1515967	A1	20050323	EP 2003-732517	20030602
EP 1515967	B1	20061102		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012446	A	20050419	BR 2003-12446	20030602
CN 1675204	A	20050928	CN 2003-818851	20030602
JP 2005533052	T	20051104	JP 2004-511297	20030602
AT 344262	T	20061115	AT 2003-732517	20030602
ES 2276072	T3	20070616	ES 2003-732517	20030602
ZA 2004009883	A	20060222	ZA 2004-9883	20041207
MX 2004PA12439	A	20050419	MX 2004-PA12439	20041209
NO 2005000063	A	20050106	NO 2005-63	20050106
US 2006160877	A1	20060720	US 2006-516777	20060113
PRIORITY APPLN. INFO.:			DE 2002-10225536	A 20020610
			DE 2002-10257078	A 20021206
			DE 2002-10257537	A 20021210
			DE 2003-10305922	A 20030213
			WO 2003-EP5735	W 20030602

OTHER SOURCE(S): MARPAT 140:42022

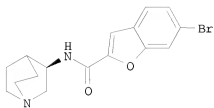
GI



I



II



III

AB The invention relates to the novel 2-heteroaryl carboxamides I [R1 = 1-azabicyclo[2.2.2]oct-3-yl, (optionally replaced via the nitrogen atom by a group selected from the family C1-4-alkyl, benzyl and oxy); R2 = H, C1-6-alkyl; R3 = H, halogen, C1-6-alkyl; R4 = H, halogen, CN, NH2, CF3, OCF3, C1-6-alkyl, C1-6-alkylcarbonyl, C1-6-alkylamino, CHO, CO2H, C1-6-alkoxy, C1-6-alkoxycarbonyl, C1-6-alkylthio, C1-6-alkylcarbonylamino, C1-6-alkylaminocarbonyl, C1-4-alkylsulfonylamino, C3-8-cycloalkylcarbonylamino, C3-6-cycloalkylaminocarbonyl, pyrrolyl, C1-6-alkylaminocarbonyl, heterocyclylcarbonyl, heterocyclylcarbonylamino, heteroarylcarbonylamino, OH, Ph, heterocyclyl; A = O, S; the ring B = benzo or pyrido (optionally replaced by the groups from the family of halogen, cyano, formyl, trifluoromethyl, trifluoromethoxy, nitro, amino, C1-6-alkyl and C1-6-alkoxy); E = C:C, aryl and heteroaryl, (wherein aryl and heteroaryl may be replaced by groups from the family of halogen, cyano, trifluoromethyl, trifluoromethoxy, nitro, amino, C1-6-alkoxy and C1-6-alkyl)] and to the solvates, salts or solvates of salts of said compds. Thus, carboxamide II was prepared from carboxamide III via coupling with 2-(HOCH2)C6H4B(OH)2 in aqueous DMF containing NaOH and catalytic [1,1'-bis(diphenylphosphino)ferrocene]palladium(II) chloride. The invention also relates to the use of said compds. in the production of drugs for and treatment and/or the prophylaxis of diseases for improving perception, power of concentration, learning power and/or retentiveness of memory. The affinity of I for α -nicotinic acetylcholine receptor (via inhibition of [3H]Methyllycaconitine binding in rat brain membranes) was determined [K1 = 1.6 nM {I·HCl; R1 = (R)-1-azabicyclo[2.2.2]oct-3-yl, R2 = R3 = H, A = S, B = benzo; 7-ER4 = 4-(hydroxymethyl)phenyl}; Ki = <1 nM {I·2HCl; R1 = (R)-1-azabicyclo[2.2.2]oct-3-yl, R2 = R3 = H, A = S, B = benzo; 7-ER4 = 2-(aminomethyl)phenyl}; Ki = <0.1 nM {I·HCl; R1 = (R)-1-azabicyclo[2.2.2]oct-3-yl, R2 = R3 = H, A = S, B = benzo; 7-ER4 = 3-carboxyphenyl}; Ki = 3 nM {I·HCl; R1 = (R)-1-azabicyclo[2.2.2]oct-3-yl, R2 = R3 = H, A = O, B = benzo; 7-ER4 = 3-(cyclopropylaminocarbonyl)phenyl}].

IT 634905-02-5P 634905-03-6P 634905-04-7P

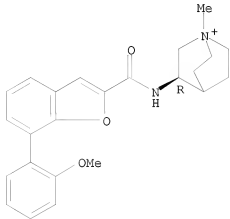
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-heteroaryl carboxamides for the treatment and/or the prophylaxis of diseases effecting memory and perception)

RN 634905-02-5 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[7-(2-methoxyphenyl)-2-benzofuranyl]carbonyl]amino]-1-methyl-, chloride, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

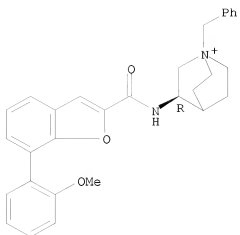


● Cl⁻

RN 634905-03-6 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[7-(2-methoxyphenyl)-2-benzofuranyl]carbonyl]amino]-1-(phenylmethyl)-, bromide, (3R)- (9CI) (CA INDEX NAME)

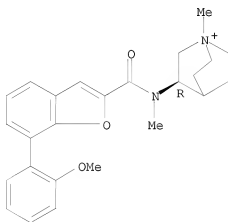
Absolute stereochemistry.



RN 634905-04-7 CAPLUS

CN 1-Azoniabicyclo[2.2.2]octane, 3-[[[7-(2-methoxyphenyl)-2-benzofuranyl]carbonyl]methylamino]-1-methyl-, chloride, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 18:57:40 ON 19 FEB 2008)

FILE 'REGISTRY' ENTERED AT 18:58:17 ON 19 FEB 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 173 S L1 FULL

FILE 'CAPLUS' ENTERED AT 18:59:16 ON 19 FEB 2008

L4 6 S L3 FULL

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

42.30

221.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-4.80

-4.80

STN INTERNATIONAL LOGOFF AT 19:11:27 ON 19 FEB 2008